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Grad's 13 Moment Equations in a Modified Form

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We describe a hierarchy of formal expansions that represent the Fourier transform of a solution of the Boltzmann equation. The constructed approximations are based on the family of weighted Taylor expansions. The first two representations correspond to the Maxwellian and to the Gaussian expansions. The third representation has a weight that generalizes the Gaussian and it depends on the first 13 moments of the Boltzmann density f. It can be shown that this weight is Galilean invariant and it is close to the Gaussian, providing that the heat fluxes are not too large. The 13 moment weight yields a revised form of Grad's 13 moment expansion for the Boltzmann equation. In search for the entropy dissipation inequality, we also examine the relation between Levermore's 14 moment and Grad's 13 moment expansion. First, we show that the coefficients of the Godunov potential are described by a system of partial differential equations, with coefficients that depend on the Fourier transform of the Levermore's density f_Λ. Then, we argue that the same Taylor expansion exploited in the Grad's scheme can be used to approximate Levermore's 14 moment density. We also show that the weighted Taylor expansions are related to a formal solution of the Hamburger problem.

KEY WORDS: Boltzmann equation, Grad moment equations, weighted Taylor expansion, Godunov potential, Hamburger moment problem

INTRODUCTION

We examine a family of expansions that represent the density $f(t, x, \xi)$ which solves the Boltzmann equation. In particular, we construct different, weighted Taylor expansions of $\widehat{f}(t, x, k)$, the Fourier transform of $f(t, x, \xi)$. Each weight corresponds to a different, finite sequences of moments of $f(t, x, \xi)$. The first two representations of $\widehat{f}(t, x, k)$ correspond to the Maxwellian and to the Gaussian. The Taylor expansion with the Maxwellian weight corresponds to the Grad

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expansion of $f(t, x, \xi)$ in a series of Hermite polynomials (see Refs. 10, 11). The Gaussian weight alone corresponds to Levermore's "10 moment closure" (see Refs. 16, 17). The third weight depends on the traditional 13 moments of $f(t, x, \xi)$ and it seems to be new. We point out that the Maxwellian appears in our expansion coincidentally, without any reference to Boltzmann equation. This fact seems to be related to the Fourier transform itself and to the condition of Galilean invariance imposed on the weighted Taylor expansions.

By continuing with our algorithm, we also construct the next, 20 moment weight that depends on all third order moments of $f(t, x, \xi)$. As soon as we try to incorporate the moments of the fourth order, our algorithm becomes irregular. The source of that irregularity is related to the specific criterion of the optimum that, together with the Galilean invariance, is at the core of our algorithm: we compute our weights by minimizing the pointwise error term in the Taylor expansions. This criterion alone does not guarantee that the resulting weights have an inverse Fourier transform—a necessary condition for self consistency of our scheme. In order to preserve this property, for all possible choices of the fourth moments, we are forced to exclude them from the exponent of the weight. Consequently, for all prescribed, finite sequences of moments of $f(t, x, \xi)$ that contain moments of fourth order and higher, our expansion becomes of a mixed type: all odd order moments enter the exponent of the weight and the even order moments go into the coefficients of the power series. We must admit that our analysis of this phenomenon is less than rigorous. However, we think that there exists an intriguing connection between the weighted Taylor series, the Chapman-Enskog expansion (see Refs. 5, 11, 13), the Hamburger moment problem (see Ref. 21) and the Central Limit Theorem; all studied by Fourier transform.

The paper is divided into 3 sections. In Sec. 1 we describe the construction of the weighted Taylor expansion based on the finite sequences of moments that, conceptually, we assume to be known. In our formulation of the problem, we owe a great deal to Levermore's paper[(16)] that emphasizes Galilean invariance of all potential approximations of the Boltzmann equation (see also Refs. 13, 15, 19).

In Sec. 2 we describe the 13 moment closure scheme that exploits the 13 moment weight of the Taylor expansion. The weights that we describe do not have an explicit inverse Fourier transform. Thus, it is essential that we have the Fourier transform of the Boltzmann equation itself. Its derivation and analysis can be found in Ref. 1 and in Bobylev's paper.[(2)] In Appendix III, we also describe an alternative derivation that goes well with the hard sphere model.

The choice of the closure scheme is somewhat arbitrary. The first choice can be based on the remainder formula for the finite Taylor expansion. We also describe second interpretation of the closure scheme that attempts to relate the 13 moment expansion to Levermore's 14 moment approximation of the density $f(t, x, \xi)$. We make this choice having in mind the entropy dissipation inequality, that is not a natural part of our approximation. However, we would like to stress that in either case, we end up with the same evolution equations, computed by the same algorithm.

As the result of our computations, we modify Grad's 13 moment equation. The most pronounce differences appear in the equations which describe the evolution of the heat fluxes. We obtain different nonlinear terms than those found in Grad's equations.

Finally, in Sec. 3 we examine Levermore's 14 moment density itself. First, we show that Levermore's centered density $f_\Lambda[\xi]$ is independent of the macroscopic velocity u of the gas. This is the key compatibility condition that we need in order to reconcile the 14 moment approximation of the Boltzmann equation with the Grad 13 moment expansion. Secondly, we demonstrate that the coefficients of the Godunov potential are described by a system of partial differential equations with coefficients that are the k derivatives of $\widehat{f_\Lambda}[k]$. We argue that those equations should, in principle, be solvable by the same, weighted Taylor expansion that modifies the Grad equations. We don't pursue this idea further since its scope is certainly beyond the horizon of a single paper.

Lastly, we wish to point out that, although we ignore the error terms in the weighted Taylor expansion and in the Pizzetti formula, both expansions have their finite counterparts, as described in Appendix I and II.

CONVENTIONS AND NOTATION

We freely use the standard multi-index notation. We also use the Einstein's summation convention. We have two different symbols for the functions of t, x, v, ξ or k. The round parentheses indicate that we list all the independent arguments of f or $\widehat{f}$. The square parentheses indicate that we list only the variables that matter in a particular context. Thus, for example, we may write $f(t, x, \xi)$ or $f[\xi]$ depending on the circumstances. Sometimes we skip the variables altogether and just write f.

1. APPROXIMATION OF THE BOLTZMANN DENSITY

We consider a positive density $F(t, x, v)$ that solves the Boltzmann equation for the gas of hard spheres,

$$\frac{\partial F}{\partial t} + v \cdot \nabla_x F + g \cdot \nabla_v F = \frac{1}{\lambda} Q\,[F, F]\,, \quad t > 0, \quad x \in \mathrm{E}^3, \quad v \in \mathrm{E}^3. \quad (1.1)$$

We wish to construct an approximate solution of Eq. (1.1) that is based on finite number of moments of the density $F(t, x, v)$. In particular, we are interested in the 13 moment approximation of F that could improve Grad's approximation as described in Refs. 10, 11. For the macroscopic density ρ and for the macroscopic velocity u,

$$\rho = \int_{E^3} dv F[v], \quad \rho u_a = \int_{E^3} dv v_a F[v], \tag{1.2}$$

define the centered density $f[\xi]$ by the formula,

$$f[\xi] = F[\xi + u], \quad \xi = v - u. \tag{1.3}$$

We introduce the stress tensor θ_{ab} and the heat flux χ_a,

$$\rho\theta_{ab} = \int_{E^3} d\xi\, \xi_a \xi_b\, f[\xi], \quad \rho\chi_a = \int_{E^3} d\xi\, \xi_a \langle \xi | \xi \rangle\, f[\xi], \tag{1.4}$$

that differ from their traditional counterparts by a factor ρ. If σ stands for the Cauchy stress, q is the standard heat flux and θ is the temperature then,

$$\sigma_{ab} = \rho\theta_{ab}, \quad q_a = \frac{1}{2}\rho\chi_a, \quad \theta = \frac{1}{3}\frac{\sigma_{nn}}{\rho} \equiv \frac{p}{\rho}. \tag{1.5}$$

We define the Fourier transform of $F[v]$ by the integral,

$$\widehat{F}[k] = \int_{E^3} dv e^{-i\langle k|v\rangle} F[v]. \tag{1.6}$$

Upon the change of variables, $v = \xi + u$, Eq. (1.6) yields the relation,

$$\widehat{F}[k] = e^{-i\langle k|u\rangle} \widehat{f}[k], \tag{1.7}$$

where $\widehat{f}[k]$ stands for the Fourier transform of $f[\xi]$,

$$\widehat{f}[k] = \int_{E^3} d\xi e^{-i\langle k|\xi\rangle} f[\xi]. \tag{1.8}$$

The moments of $f[\xi]$, that describe the macroscopic properties of gas, can be expressed in terms of the derivatives of $\widehat{f}[k]$ at $k = 0$,

$$\widehat{f}[0] = \rho, \quad \partial_a \widehat{f}[0] = 0, \quad \partial_a\partial_b \widehat{f}[0] = -\rho\theta_{ab}, \quad \partial_a \Delta \widehat{f}[0] = i\rho\chi_a. \tag{1.9}$$

As it is discussed in Levermore's paper,[16] solutions of the Boltzmann equation, over the whole space, must be invariant under Galilean group of transformations. That is, for any orthogonal transformation $\mathcal{O}$:$E^3 \longrightarrow E^3$ and for any constant vector u_0 the mappings,

$$F(t, x, v) \longrightarrow F(t, x - tu_0, v - u_0), \quad F(t, x, v) \longrightarrow F(t, \mathcal{O}x, \mathcal{O}v), \tag{1.10}$$

must transform any solution of Eq. (1.1) into another solution of the Boltzmann equation. In terms of the Fourier transform Eqs. (1.10) yield two mappings,

$$\widehat{F}(t, x, k) \longrightarrow e^{-i\langle k|u_0\rangle} \widehat{F}(t, x - tu_0, k), \quad \widehat{F}(t, x, k) \longrightarrow \widehat{F}(t, \mathcal{O}x, \mathcal{O}k). \tag{1.11}$$

In Appendix I we show that given a sufficiently smooth function $B[k]$, any "nice" function $\widehat{f}[k]$ can be expanded into a formal, weighted Taylor series,

$$\widehat{f}[k] = e^{-B[k]} \left[\widehat{f}[0] + \sum_{N=1}^{\infty} \sum_{|\alpha|=N} L^{\alpha} \widehat{f}[0] \frac{k^{\alpha}}{\alpha!} \right], \tag{1.12}$$

where,

$$L^{\alpha} = L_1^{\alpha_1} L_2^{\alpha_2} L_3^{\alpha_3}, \quad L_a \widehat{f}[k] = \partial_a \widehat{f}[k] + \partial_a B[k] \, \widehat{f}[k]. \tag{1.13}$$

Assuming that $\widehat{f}[k]$ represents a solution of the Boltzmann equation and $B[k]$ a polynomial in k, we impose two conditions on $B[k]$. First of all, $B[\mathcal{O}k]$ must be a polynomial of the same type as $B[k]$ is. Secondly, $\exp(-B[k])$ must be an integrable function over E^3 if we wish to recover $f[\xi]$ through the inverse Fourier transform of $\widehat{f}[k]$. Comparing above constraints with the definition of $\mathbb{M}$ spaces in Levermore's paper, we conclude that the first seven candidates for $B[k]$ are (see Ref. 16, p. 1037, Eq. (4.8)):

1. $B[k] = \sum_{|\alpha|\le 1} B_\alpha k^\alpha + W_0 \langle k|\, k\rangle$, —"5 *moment expansion*",
2. $B[k] = \sum_{|\alpha|\le 2} B_\alpha k^\alpha$, —"10 *moment expansion*",
3. $B[k] = \sum_{|\alpha|\le 2} B_\alpha k^\alpha + \langle N|\, k\rangle \langle k|\, k\rangle$, —"13 *moment expansion*",
4. $B[k] = \sum_{|\alpha|\le 3} B_\alpha k^\alpha$, —"20 *moment expansion*",

and

5. $B[k] = \sum_{|\alpha|\le 2} B_\alpha k^\alpha + W_0 \langle k|\, k\rangle^2$, —"14 *moment expansion*",
6. $B[k] = \sum_{|\alpha|\le 3} B_\alpha k^\alpha + W_0 \langle k|\, k\rangle^2$, —"21 *moment expansion*",
7. $B[k] = \sum_{|\alpha|\le 4} B_\alpha k^\alpha$, —"35 *moment expansion*".

In order to determine the coefficients of each $B[k]$, we proceed inductively. We start with the "5 moment expansion." We try to optimize expansion (1.12) by annihilating as many successive coefficients $L^\alpha \widehat{f}[0]$ as we can. Eq. (1.9) imply that $\widehat{f}[0] = \rho$ so $B[0] = 0$. Next, we set

$$L_a \widehat{f}[0] = \partial_a \widehat{f}[0] + \partial_a B[0] \, \widehat{f}[0] = 0. \tag{1.14}$$

By Eq. (1.9), $\partial_a \widehat{f}[0] = 0$. Thus all B_α's are zero. We are left with a single coefficient W_0. We impose the last condition,

$$\left[L_1^2 + L_2^2 + L_3^2\right] \widehat{f}[0] = 0. \tag{1.15}$$

Simple computations yield (see the formulae in Appendix I),

$$\Delta \widehat{f}[0] + 6 W_0 \widehat{f}[0] = 0. \tag{1.16}$$

Since the Laplacian Δ defines the macroscopic temperature θ according to the formula

$$\Delta \widehat{f}[0] = -\rho\theta_{aa} = -3\rho\theta, \tag{1.17}$$

we obtain $W_0 = \frac{1}{2}\theta$. Therefore expansion (1.12) is,

$$\widehat{f}[k] = \exp\left(-\frac{1}{2}\theta\langle k\,|k\rangle\right)\left[\rho + \sum_{N=1}^{\infty}\sum_{|\alpha|=N} L^{\alpha}\widehat{f}[0]\,\frac{k^{\alpha}}{\alpha!}\right], \tag{1.18}$$

$$L_a\widehat{f}[k] = \partial_a\widehat{f}[k] + \theta k_a\widehat{f}[k]\,.$$

The inverse Fourier transform of

$$\widehat{M}[k] = \rho\exp\left(-\frac{1}{2}\theta\langle k\,|k\rangle\right), \tag{1.19}$$

is the standard Maxwellian,

$$M[\xi] = \frac{\rho}{[2\pi\theta]^{\frac{3}{2}}}\exp\left(-\frac{1}{2}\theta^{-1}\langle\xi\,|\xi\rangle\right). \tag{1.20}$$

Consequently, by taking the inverse Fourier transform of expansion (1.18) we recover Grad's expansion of $f[\xi]$ into Hermite polynomials (see Refs. 10, 11).

Next, we consider the "10 moment expansion." Again, we try to annihilate successive coefficients in expansion (1.12). Conditions $\widehat{f}[0] = \rho$ and $L_a\widehat{f}[0] = 0$ imply that all B_α's, for $|\alpha| \leq 1$ vanish. We add a new condition, $L_aL_b\widehat{f}[0] = 0$. Since

$$L_aL_b\widehat{f}[0] = \partial_a\partial_b\widehat{f}[0] + \partial_a\partial_b B\,[0]\,\widehat{f}[0]\,, \tag{1.21}$$

we conclude that $\partial_a\partial_b B\,[0] = \theta_{ab}$. Therefore expansion (1.12) yields,

$$\widehat{f}[k] = \exp\left(-\frac{1}{2}\langle\theta k\,|k\rangle\right)\left[\rho + \sum_{N=3}^{\infty}\sum_{|\alpha|=N} L^{\alpha}\widehat{f}[0]\,\frac{k^{\alpha}}{\alpha!}\right], \tag{1.22}$$

$$L_a\widehat{f}[k] = \partial_a\widehat{f}[k] + \theta_{ab}k_b\widehat{f}[k]\,.$$

By taking the inverse Fourier transform of Eq. (1.22), we recover the expansion of $f[\xi]$ with respect to the Gaussian weight. The Gaussian closure was studied by Levermore in Ref. 16 and Levermore, Morokoff in Ref. 17, as a "10 moment closure." Expansion (1.22), generates a Grad-like moment approximation of the Boltzmann equation, with the Gaussian in place of the Maxwellian.

We continue our computations with the next $B[k]$,

$$B\,[k] = \sum_{|\alpha|\leq 2} B_\alpha k^\alpha + \langle N|\,k\rangle\,\langle k|\,k\rangle. \tag{1.23}$$

Following the previous pattern, we associate with every polynomial that is multiplied by the unknown coefficient B_α, an algebraic condition,

$$P_\alpha\,(k_1,k_2,k_3) \longrightarrow P_\alpha\,(L_1,L_2,L_3)\,\widehat{f}\,[0]=0. \tag{1.24}$$

Each time we obtain an equation that identifies coefficient B_α in terms of the derivatives $\partial^\beta \widehat{f}[0]$ that are listed in Eq. (1.9). In particular case of Eq. (1.23), we have the following sequence of conditions,

$$\begin{aligned}
1 &\longrightarrow \widehat{f}\,[0]=\rho \iff B\,[0]=0,\\
k_a &\longrightarrow L_a\widehat{f}\,[0]=0 \iff \partial_a B\,[0]=0,\\
k_ak_b &\longrightarrow L_aL_b\widehat{f}\,[0]=0 \iff \partial_a\partial_b B\,[0]=\theta_{ab},\\
k_a\,\langle k|\,k\rangle &\longrightarrow L_a[L_1^2+L_2^2+L_3^2]\widehat{f}\,[0]=0 \iff \partial_a\Delta B\,[0]=-i\chi_a.
\end{aligned} \tag{1.25}$$

Consequently,

$$B\,[k]=\frac{1}{2}\,\langle\theta k|\,k\rangle-\frac{i}{10}\,\langle\chi\,|\,k\rangle\,\langle k|\,k\rangle. \tag{1.26}$$

Therefore,

$$\widehat{f}\,[k]=\exp\left(-\frac{1}{2}\,\langle\theta k|\,k\rangle+\frac{i}{10}\,\langle\chi\,|\,k\rangle\,\langle k|\,k\rangle\right)\left[\rho+\sum_{N=3}^{\infty}\sum_{|\alpha|=N}L^\alpha\widehat{f}\,[0]\,\frac{k^\alpha}{\alpha!}\right],$$

$$L_a\widehat{f}\,[k]=\partial_a\widehat{f}\,[k]+[\theta_{ab}k_b-\frac{i}{10}\chi_a\,\langle k|\,k\rangle-\frac{i}{5}\,\langle\chi\,|\,k\rangle k_a]\,\widehat{f}\,[k]\,. \tag{1.27}$$

We notice that expansion (1.27) can formally be inverted, term by term, using the Fourier transform. However, the oscillatory term in the weight makes an explicit computations difficult. Still, we wish to know whether the new weight,

$$\widehat{w}\,[k]=\exp\left(-\frac{1}{2}\,\langle\theta k|\,k\rangle+\frac{i}{10}\,\langle\chi\,|\,k\rangle\,\langle k|\,k\rangle\right), \tag{1.28}$$

has an inverse Fourier transform, $w\,[\xi]$, that is real and positive. Regrettably, this is not quite the case. We examine the function,

$$\widehat{w}_s\,[k]=\exp\left(-\frac{1}{2}\,\langle\theta k|\,k\rangle+is\,\langle\beta|\,k\rangle\,\langle k|\,k\rangle\right),\quad \beta=\frac{\chi}{10}. \tag{1.29}$$

Its inverse Fourier transform is given by the integral,

$$w_s\,[\xi]=\int_{E^3}\frac{dk}{[2\pi]^3}e^{i\langle k|\xi\rangle}\exp\left(-\frac{1}{2}\,\langle\theta k|\,k\rangle+is\,\langle\beta|\,k\rangle\,\langle k|\,k\rangle\right). \tag{1.30}$$

By the standard properties of the Fourier transform, $w_s[\xi]$ is a solution of the linear, dispersive, partial differential equation,

$$\frac{\partial}{\partial s} w_s[\xi] = -\beta_a \partial_a \Delta w_s[\xi], \tag{1.31}$$

with the Gaussian initial condition,

$$w_0[\xi] = [\det[2\pi\theta]]^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\left\langle \theta^{-1}\xi \,\middle|\, \xi\right\rangle\right). \tag{1.32}$$

Therefore, $w_s[\xi]$ is real for all s and it remains close to the Gaussian for small s. Consequently $w[\xi] = \mathcal{F}^{-1}(\widehat{w}[k])$ is real and close to the Gaussian for small χ. Unfortunately, $w_s[\xi]$ cannot be positive. Trivial expansion of the integral (1.30) yields,

$$w_s[\xi] = w_0[\xi][1 + sP_1(\xi) + \cdots], \tag{1.33}$$

where $P_1(\xi)$ is a cubic polynomial in ξ. Thus $w_s[\xi]$ must, eventually, become negative for any $s \neq 0$. In fact, for ξ in R any weight past the Gaussian cannot be positive by the Marcinkiewicz theorem (see Ref. 18). The problem of finding an asymptotic behavior of $w_s[\xi]$ as $s \longrightarrow \infty$ belongs to the theory of oscillatory integrals (see Ref. 22) which shows that $w_s[\xi]$ picks up oscillatory terms for large s. Thus any computation based on the approximation,

$$\widehat{f}[k] \approx \rho \exp\left(-\frac{1}{2}\langle\theta k|\,k\rangle + \frac{i}{10}\langle\chi\,|\,k\rangle\,\langle k|\,k\rangle\right), \tag{1.34}$$

becomes suspect for large heat fluxes q_a.

The "20 moment expansion" generates a legitimate weight that generalizes our result for "13 moment expansion." We replace the last Eq. (1.25) by a modified condition,

$$\begin{aligned} k^\alpha \longrightarrow L^\alpha \widehat{f}[0] = 0 &\iff \partial^\alpha B[0] = \chi_\alpha, \\ \rho\chi_\alpha \;=\; \frac{1}{i}\partial^\alpha \widehat{f}[0] &= \int_{E^3} d\xi \xi^\alpha f[\xi], |\alpha| = 3. \end{aligned} \tag{1.35}$$

We obtain generalized expansion (1.27),

$$\widehat{f}[k] = \exp\left(-\frac{1}{2}\langle\theta k|\,k\rangle + i\sum_{|\alpha|=3}\chi_\alpha\frac{k^\alpha}{\alpha!}\right)\left[\rho + \sum_{N=4}^{\infty}\sum_{|\alpha|=N} L^\alpha \widehat{f}[0]\,\frac{k^\alpha}{\alpha!}\right]. \tag{1.36}$$

We notice that, the inclusion of all cubic monomials in $B[k]$ results in an error term of order $\mathcal{O}(k^4)$, while expansion (1.27) has an error term of order $\mathcal{O}(k^3)$, like the Gaussian expansion.

It is possible to investigate Taylor expansion for the remaining polynomials $B[k]$. We consider the "14 moment expansion." We try to extend the scheme

(1.25) by adding the next condition,

$$\langle k|\,k\rangle^2 \longrightarrow \left[L_1^2 + L_2^2 + L_3^2\right]^2 \widehat{f}\,[0] = 0 \iff W_0 = \frac{1}{5!}\left[[tr\theta]^2 + 2tr\theta^2 - \mu\right],$$
$$\mu = \Delta^2 \widehat{f}\,[0] = \int_{\mathrm{E}^3} d\xi\, \langle\xi\,|\,\xi\rangle^2 f\,[\xi]\,. \tag{1.37}$$

Unfortunately, there is no guarantee that $W_0 \geq 0$. Consequently the "14 moment expansion" corresponds to a weight that may or may not have an inverse Fourier transform. However, the weighted Taylor expansion remains valid for small k's.

It is still a realistic undertaking to study 21 and 35 "moment expansions." In the first case, we recover the same W_0 as for the "14 moment expansion." Thus the resulting weight cannot, in general be Fourier inverted; it remains valid locally, for small k. There are similar difficulties with "35 moment expansion." The dominant, quartic monomials behave like W_0 and the corresponding expansion fails, in general, to have a Fourier inverse.

One may ask what happens next, for B's that contain monomials of degree larger than 4. We do not know the precise answer since the resulting formulas for $L^\alpha \widehat{f}\,[k]$'s become quite complex. However, one can study a one-dimensional case with greater precision, under the condition that the weighted expansion has a formal Fourier inverse. Based on such an analysis, one can write a hypothetical expansion that has the following form,

$$\widehat{f}\,[k] = \exp\left(-\frac{1}{2}\theta k^2 + i\Omega_N\,[k]\right)\left[\rho + \sum_{j=2}^{N} L_N^{2j}\widehat{f}\,[0]\,\frac{k^{2j}}{(2j)!} + R_N\,[k]\right]. \tag{1.38}$$

$\Omega_N\,[k]$ stands for an odd, real polynomial in k,

$$\Omega_N\,[k] = \omega_3 k^3 + \omega_5 k^5 + \omega_7 k^7 + \cdots + \omega_{2N+1} k^{2N+1}. \tag{1.39}$$

whose coefficients ω_{2j+1} can be computed from the sequence of conditions,

$$k^{2j+1} \longrightarrow L_N^{2j+1}\widehat{f}\,[0] = 0, \quad j = 1, 2, \ldots, N. \tag{1.40}$$

The key future of the computation is the fact that $D\widehat{f}\,[0] = 0$. This condition seems to separate the odd and the even moments of $f\,[\xi]$. The odd moments enter the formulae for ω_{2j+1}. The even moments end up in the coefficients $L_N^{2j}\widehat{f}\,[0]$. Moreover, it is possible to let $N \longrightarrow \infty$ since the inductive character of the computations, like in the ordinary Taylor expansion, makes ω_n's and $L^n\widehat{f}\,[0]$'s, for n smaller than N, independent of N. In this case, we obtain the expansion,

$$\widehat{f}\,[k] = \exp\left(-\frac{1}{2}\theta k^2 + i\Omega\,[k]\right)\left[\rho + \sum_{j=0}^{\infty} L^{2j+4}\widehat{f}\,[0]\,\frac{k^{2j+4}}{(2j+4)!}\right]. \tag{1.41}$$

The coefficients ω are determined by the conditions,

$$L^{2j+1}\widehat{f}[0] = 0, \quad j = 1, 2, 3, \ldots,$$
$$\Omega[k] = \sum_{m=1}^{\infty} \omega_{2m+1} k^{2m+1}, \tag{1.42}$$

providing that

$$L\widehat{f}[k] = D\widehat{f}[k] + [\theta k - iD\Omega[k]]\,\widehat{f}[k]. \tag{1.43}$$

There exists an intriguing possibility that Eq. (1.41) represents a formal solution of the Hamburger problem, where one attempts to recover the formula for $f[\xi] \geq 0$ knowing all the moments of f (see Simon's review Ref. 21). Moreover, the formula (1.41) can be used to provide intuitive arguments supporting the Central Limit Theorem.

We could also write a three dimensional analog of Eq. (1.41) by setting,

$$\widehat{f}[k] = \exp\left(-\frac{1}{2}\langle\theta k|\, k\rangle + i\Omega[k]\right)[\rho + \Upsilon[k]],$$
$$\Omega[k] = \sum_{N=1}^{\infty} \sum_{|\alpha|=2N+1} \omega_\alpha k^\alpha, \quad \Upsilon[k] = \sum_{N=2}^{\infty} \sum_{|\alpha|=2N} L^\alpha \widehat{f}[0]\,\frac{k^\alpha}{\alpha!}. \tag{1.44}$$

The ω_α's would be defined by the conditions,

$$L^\alpha \widehat{f}[0] = 0, \quad |\alpha| = 2N+1, \quad N = 1, 2, 3, \ldots$$
$$L_a \widehat{f}[k] = \partial_a \widehat{f}[k] + [\theta_{ab} k_b - i\partial_a \Omega[k]]\widehat{f}[k]. \tag{1.45}$$

In order to justify this analogy, we would have to demonstrate that $\Omega[k]$ and $\Upsilon[k]$ are real. Then, we would have to establish that $\Omega[k]$ depends on the odd moments of f and to show that $\Upsilon[k]$ contains the moments of the even order alone. Next, we would have to prove that expansion (1.44) converges. In that case, as a reward, we could establish that the Hamburger problem in E^3, for $f \geq 0$, is equivalent to a quantitative version of the Chapman-Enskog hypothesis (see Refs. 4, 5, 11), examined on the Fourier side of the Boltzmann equation.

2. GRAD'S MODIFIED 13 MOMENT CLOSURE

The Fourier transform of the Boltzmann equation has the following form (see Refs. 1, 2 and Appendix III),

$$\frac{\partial \widehat{F}}{\partial t} + i\frac{\partial}{\partial x_a}\partial_a \widehat{F} = \frac{1}{\lambda}\widehat{Q}[\widehat{F}, \widehat{F}], \quad \partial_a(\cdot) = \frac{\partial(\cdot)}{\partial k_a}. \tag{2.1}$$

We set

$$\widehat{F}(t,x,k) = e^{-i\langle k|u(t,x)\rangle}\widehat{f}(t,x,k), \tag{2.2}$$

and we express Eq. (2.1) in terms of $\widehat{f}$. Since

$$\widehat{Q}[\widehat{F},\widehat{F}] = e^{-i\langle k|u(t,x)\rangle}\widehat{Q}[\widehat{f},\widehat{f}], \tag{2.3}$$

we obtain,

$$\begin{aligned}&\frac{D\widehat{f}}{Dt} + \frac{\partial u_a}{\partial x_a}\widehat{f} + i\frac{\partial}{\partial x_a}\partial_a\widehat{f} - i\frac{Du_a}{Dt}k_a\widehat{f} + \frac{\partial u_b}{\partial x_a}k_b\partial_a\widehat{f} = \frac{1}{\lambda}\widehat{Q}[\widehat{f},\widehat{f}],\\ &\frac{D(\cdot)}{Dt} = \frac{\partial(\cdot)}{\partial t} + u_n\frac{\partial(\cdot)}{\partial x_n},\end{aligned} \tag{2.4}$$

with the side condition on $\widehat{f}$,

$$\partial_a\widehat{f}(t,x,0) = 0. \tag{2.5}$$

We point out that all weighted Taylor expansions, by construction, satisfy Eq. (2.5).

In the previous section, we constructed different expansions of a single function $\widehat{f}$ that represents a formal solution of the Boltzmann equation. The first two weights, the Maxwellian and the Gaussian, fit Levermore's moment closure hierarchy that is studied on the Fourier side of the Boltzmann equation. The third weight, that corresponds to 13 moment expansion, does not belong to that hierarchy, since its inverse Fourier transform is not positive. Thus, if we wish to use the third weight to approximate the solution of the Boltzmann equation, we must construct a closure scheme for $\widehat{F_*}[k]$ (see Eq. (1.27)),

$$\begin{aligned}&\widehat{F_*}[k] = e^{-i\langle k|u_*\rangle}\widehat{f_*}[k],\\ &\widehat{f_*}[k] = \rho_*\exp\left(-\frac{1}{2}\langle\theta_* k|\, k\rangle + \frac{i}{10}\langle\chi_*|\, k\rangle\langle k|\, k\rangle\right).\end{aligned} \tag{2.6}$$

The first possibility is to consider the finite version of expansion (1.27),

$$\widehat{f}[k] = \exp\left(-\frac{1}{2}\langle\theta k|\, k\rangle + \frac{i}{10}\langle\chi|\, k\rangle\langle k|\, k\rangle\right)[\varrho + R_3[k]], \tag{2.7}$$

with the explicit error term $R_3[k]$ described in Appendix I. The principal part of the ordinary Taylor expansion of Eq. (2.7) depends on 13, linearly independent monomials k^α,

$$1,\ k_a,\ k_ak_b,\ k_ak_sk_s. \tag{2.8}$$

Those monomials are in 1:1 correspondence with the macroscopic quantities computed from the set of conditions:

$$\begin{aligned} &\widehat{f}\,[0] = \rho, \quad \partial_a \widehat{f}\,[0] = 0, \\ &\partial_a \partial_b \widehat{f}\,[0] = -\rho\theta_{ab} = -\sigma_{ab}, \quad \partial_a \Delta \widehat{f}\,[0] = i\rho\chi_a = i2q_a. \end{aligned} \tag{2.9}$$

To pursue this duality further, we substitute expansion (2.7) into the Boltzmann equation (2.4) and we apply to the resulting equation the sequence of 13 differential operators evaluated at $k = 0$,

$$1\,(\cdot)\,[0]\,, \quad \partial_a\,(\cdot)\,[0]\,, \quad \partial_a\partial_b\,(\cdot)\,[0]\,, \quad \partial_a\Delta\,(\cdot)\,[0]\,. \tag{2.10}$$

Next, we set $R_3 \equiv 0$ and we arrive at the system of 13 equations for the 13 moments of $f\,[\xi]$.

The second possibility is to consider Eq. (1.27) as a Taylor expansion of the Fourier transform of Levermore's 14 moment density (for μ see Eq. (1.37)),

$$\widehat{F}_\Lambda\,[k] \equiv \widehat{F}_\Lambda\,[k, u_*, \rho_*, \theta_*, \chi_*, \mu_*]\,. \tag{2.11}$$

In the next section, we show that $\widehat{F}_\Lambda$ factors into a product,

$$\widehat{F}_\Lambda\,[k] = e^{-i\langle k|u_*\rangle}\,\widehat{f}_\Lambda\,[k]\,, \tag{2.12}$$

where $\widehat{f}_\Lambda$ is independent of the macroscopic velocity u_*; a property that is also shared by expansion (1.27). Consequently, we may write,

$$\widehat{f}_\Lambda\,[k] = \exp\left(-\frac{1}{2}\,\langle\theta_* k|\,k\rangle + \frac{i}{10}\,\langle\chi_*|\,k\rangle\,\langle k|\,k\rangle\right)\left[\rho_* + \sum_{N=3}^{\infty}\sum_{|\alpha|=N} L^\alpha \widehat{f}_\Lambda\,[0]\,\frac{k^\alpha}{\alpha!}\right], \tag{2.13}$$

where all the coefficients $L^\alpha \widehat{f}_\Lambda\,[0]$ depend on $\rho_*, \theta_*, \chi_*, \mu_*$ alone. If we knew how to compute the remaining moments of $f_\Lambda\,[\xi]$, then we could substitute expansion (2.13) into Levermore's moment equations and recover their Grad-like approximation. Since we have at our disposal only the weight of the Levermore's expansion, we can substitute $\widehat{F}_*$ into his first 13 equation and we can delete the 14-th equation that must contain μ_*. As the result of this procedure, we end up pursuing Levermore's scheme on the Fourier side of the Boltzmann equation, with the truncated $\widehat{F}_\Lambda$ and without his last equation. The resulting scheme is identical with the previous one.

In order to implement the closure scheme, we differentiate the Boltzmann equation with respect to k. First we evaluate Eq. (2.4) at $k = 0$,

$$\frac{D\rho}{Dt} + \frac{\partial u_a}{\partial x_a}\rho = 0. \tag{2.14}$$

Next, we apply a sequence of 12 differential operators $\partial_s(\cdot)$, $\partial_s\partial_r(\cdot)$, $\partial_m\Delta(\cdot)$, to Eq. (2.4), we set $k = 0$ and we obtain,

$$\rho\frac{Du_s}{Dt} + \frac{\partial\sigma_{as}}{\partial x_a} = 0,$$

$$\frac{D\sigma_{rs}}{Dt} + \frac{\partial u_a}{\partial x_a}\sigma_{rs} + \frac{\partial u_r}{\partial x_a}\sigma_{as} + \sigma_{ra}\frac{\partial u_s}{\partial x_a} - i\frac{\partial}{\partial x_a}\partial_a\partial_r\partial_s\widehat{f}[0]$$
$$= -\frac{1}{\lambda}\partial_a\partial_b\widehat{Q}[\widehat{f},\widehat{f}][0],$$

$$\frac{Dq_m}{Dt} + \frac{\partial u_a}{\partial x_a}q_m + \frac{\partial u_m}{\partial x_a}q_a + \sigma_{ms}\frac{Du_s}{Dt} + \frac{1}{2}\frac{Du_m}{Dt}\sigma_{ss} + \frac{\partial u_s}{\partial x_a}\left[i^{-1}\partial_a\partial_s\partial_m\widehat{f}[0]\right]$$
$$+\frac{\partial}{\partial x_a}\left[\frac{1}{2}\partial_a\partial_m\Delta\widehat{f}[0]\right] = \frac{1}{\lambda}\frac{1}{2i}\partial_m\Delta\widehat{Q}[\widehat{f},\widehat{f}][0]. \tag{2.15}$$

Our closure scheme implies that we have to substitute in place of the true $\widehat{f}$, its approximation $\widehat{f}_*$ given by Eq. (2.6). We must also identify the macroscopic quantities defined through Eq. (2.9) with their approximate, dressed in stars, macroscopic counterparts. By construction, Eq. (2.9) are consistent with the formula for $\widehat{f}_*$. Finally, we must identify u with u_*. After all that, we drop the stars, we write Eq. (2.15) as they stand, and we pretend that the true $\widehat{f}$ is given by the formula (2.6). Now, we compute,

$$i^{-1}\partial_a\partial_s\partial_m\widehat{f}[0] = \frac{2}{5}\left[q_a\delta_{sm} + q_m\delta_{as} + q_s\delta_{am}\right],$$
$$\frac{1}{2}\partial_a\partial_m\Delta\widehat{f}[0] = \frac{3}{2}\theta\sigma_{am} + \frac{1}{\rho}\sigma_{as}\sigma_{sm}. \tag{2.16}$$

Next, we set

$$\Xi_{ab} = -\partial_a\partial_b\widehat{Q}[\widehat{f},\widehat{f}][0], \quad \Theta_m = \frac{1}{2i}\partial_m\Delta\widehat{Q}[\widehat{f},\widehat{f}][0]. \tag{2.17}$$

After standard algebraic manipulations, we arrive at the full set of 13 evolution equations,

$$\frac{D\rho}{Dt} + \frac{\partial u_a}{\partial x_a}\rho = 0,$$

$$\rho\frac{Du_m}{Dt} + \frac{\partial\sigma_{am}}{\partial x_a} = 0,$$

$$\frac{D\sigma_{mn}}{Dt} + \frac{\partial u_a}{\partial x_a}\sigma_{mn} + \frac{\partial u_m}{\partial x_a}\sigma_{an} + \sigma_{ma}\frac{\partial u_n}{\partial x_a} + \frac{2}{5}\left[\frac{\partial q_a}{\partial x_a}\delta_{mn} + \frac{\partial q_m}{\partial x_n} + \frac{\partial q_n}{\partial x_m}\right] = \frac{1}{\lambda}\Xi_{mn},$$

$$\frac{Dq_m}{Dt} + \frac{7}{5}\frac{\partial u_a}{\partial x_a}q_m + \frac{7}{5}\frac{\partial u_m}{\partial x_a}q_a + \frac{2}{5}\frac{\partial u_a}{\partial x_m}q_a + \frac{3}{2}\sigma_{ma}\frac{\partial\theta}{\partial x_a} + \sigma_{ab}\frac{\partial}{\partial x_a}\left[\frac{\sigma_{bm}}{\rho}\right] = \frac{1}{\lambda}\Theta_m. \tag{2.18}$$

Moreover, by taking the trace of the second equation we recover the balance of energy, $\Xi_{mm} = 0$,

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + D_{ab}\sigma_{ab} + \frac{\partial q_a}{\partial x_a} = 0,$$

$$D_{ab} = \frac{1}{2}\left[\frac{\partial u_a}{\partial x_b} + \frac{\partial u_b}{\partial x_a}\right], \quad \theta = \frac{p}{\rho} = \frac{1}{3}\frac{\sigma_{aa}}{\rho}. \tag{2.19}$$

We are still left with the task of computing Ξ_{ab} and Θ_m. In Appendix IV we show that the collision operator $\widehat{Q}[\widehat{f}, \widehat{f}]\,[k]$ can be expanded into a quasi-power series whose first term is

$$\widehat{Q}_1[\widehat{f}, \widehat{f}]\,[k] = \frac{1}{\pi}\int_{\mathrm{E}^3} \frac{dw}{\|w\|^2}\left[\sum_{|\alpha|=2} \frac{k^\alpha}{\alpha!}\frac{\partial^\alpha \psi}{\partial^\alpha w}\,[k, w] - \frac{\|k\|^2}{3!}\Delta_w \psi\,[k.w]\right]. \tag{2.20}$$

It is also true that for any $\widehat{f}$

$$\widehat{Q}[\widehat{f}, \widehat{f}]\,[k] = \widehat{Q}_1[\widehat{f}, \widehat{f}]\,[k] + \mathcal{O}\left(k^4\right). \tag{2.21}$$

Therefore, up to the third order, at $k = 0$, all derivatives of $\widehat{Q}$ and $\widehat{Q}_1$ are the same. Hence, Ξ_{ab} and Θ_m can be computed from the formula,

$$\widehat{Q}_1[\widehat{f}, \widehat{f}]\,[k] = \frac{1}{2}k_m k_n P_{mn}\,[k] - \frac{1}{6}k_m k_m P_{nn}\,[k],$$

$$P_{mn}\,[k] = \frac{1}{\pi}\int_{\mathrm{E}^3} \frac{dw}{\|w\|^2}\frac{\partial}{\partial w_m}\frac{\partial}{\partial w_n}\psi\,[k, w],$$

$$\psi\,[k, w] = \Delta_w \varphi\,[k, w], \quad \varphi\,[k, w] = \widehat{f}\left[\frac{1}{2}k + \frac{1}{2}w\right]\widehat{f}\left[\frac{1}{2}k - \frac{1}{2}w\right]. \tag{2.22}$$

Eq. (2.6) implies that,

$$P_{mn}\,[k] = \frac{1}{\pi}\int_{\mathrm{E}^3} \frac{dw}{\|w\|^2}\Delta_w \frac{\partial}{\partial w_m}\frac{\partial}{\partial w_n}\exp\left(-E\,[k, w]\right). \tag{2.23}$$

The exponent $E\,[k, w]$ stands for the following polynomial,

$$E\,[k, w] = \frac{1}{4}\langle \theta k|\, k\rangle + \frac{1}{4}\langle \theta w|\, w\rangle$$
$$-\frac{i}{40}\langle \chi\,|\, k\rangle\left[\langle k|\, k\rangle + \langle w|\, w\rangle\right] - \frac{i}{20}\langle \chi\,|\, w\rangle\,\langle k|\, w\rangle. \tag{2.24}$$

Straightforward differentiation yields,

$$\begin{aligned}
\Sigma_{ab} &= P_{ab}\,[0]\,,\\
\Xi_{ab} &= -\partial_a \partial_b \widehat{Q}\,[0] = \frac{1}{3}\delta_{ab}\Sigma_{nn} - \Sigma_{ab},\\
\Theta_m &= \frac{1}{2i}\partial_m \Delta \widehat{Q}\,[0] = \frac{1}{i}\partial_n P_{nm}\,[0]\,.
\end{aligned} \tag{2.25}$$

In terms of the integral formulae,

$$\begin{aligned}
\Sigma_{ab} &= \frac{\sqrt[2]{\varrho}}{\pi}\int_{\mathrm{E}^3} \frac{dw}{\|w\|^2}\Delta_w \frac{\partial}{\partial w_a}\frac{\partial}{\partial w_b}\exp\left(-\frac{1}{4}\langle \sigma w|\, w\rangle\right),\\
\Theta_m &= \frac{\sqrt[2]{\varrho}}{40\pi}\int_{\mathrm{E}^3} \frac{dw}{\|w\|^2}\Delta_w \frac{\partial}{\partial w_m}\frac{\partial}{\partial w_n}\left[2\,\langle q|\, w\rangle w_n + q_n\,\langle w|\, w\rangle\right]\\
&\quad\times \exp\left(-\frac{1}{4}\langle \sigma w|\, w\rangle\right).
\end{aligned} \tag{2.26}$$

We notice that the last equation is linear in q.

Both integrals (2.26) can be transformed into Galilean invariant form, providing that we carry out the integration using the diagonal form of $\langle \sigma w|\, w\rangle$. Details of this technique can be found in Levermore's and Morokoff's paper,(17) where they study the 10 moment closure of the general Boltzmann equation. In particular, one can show that,

$$\begin{aligned}
\Sigma &= \sqrt[2]{\varrho}\left[\gamma_2\sigma^2 + \gamma_1\sigma + \gamma_0 id\right],\\
\Theta &= \Omega\cdot q, \qquad \Omega = \sqrt[2]{\varrho}\left[\eta_2\sigma^2 + \eta_1\sigma + \eta_0 id\right].
\end{aligned} \tag{2.27}$$

The functions γ, η depend on the principal invariants of σ alone, namely,

$$I_1 = tr\,(\sigma)\,, \qquad I_2 = tr\,(ad\sigma)\,, \qquad I_3 = \det(\sigma)\,. \tag{2.28}$$

It is possible to compare Eq. (2.18) with 13 moment equations derived by Grad (see Ref. 10, pp. 366–367, Eqs. (5.17), (5.18)). Grad uses the symbols,

$$\{\varrho, u_a, P_{ab}, p_{ab}, p, RT, S_a\}\,, \tag{2.29}$$

that in our notation correspond to the sequence,

$$\{\varrho, u_a, \sigma_{ab}, \sigma_{ab} - p\delta_{ab}, p, \theta, 2q_a\}\,. \tag{2.30}$$

Comparing Grad's equations with Eq. (2.18), we conclude that conservation of mass, momentum and energy is identical in both systems. Except for Ξ tensor, Grad's evolution equations for σ_{ab}'s are also identical with ours. In Grad's work Ξ appears as,

$$-\frac{1}{\lambda}\Xi_{ab} = C\frac{\widetilde{\sigma}}{\widetilde{m}}\sqrt[2]{\varrho}\sqrt[2]{I_1}\,p_{ab}, \tag{2.31}$$

where C is a numerical constant, $\widetilde{m}$ is the mass of the molecule and $\widetilde{\sigma}$ is its diameter (see Ref. 10, p. 401, A3.54). Ξ_{ab} in our work is identical with a particular case of Levermore's and Morokoff's expression derived in Ref. 17. Finally, the evolution of the heat flux q in Grad's work is described by the equation,

$$\begin{aligned}&\frac{Dq_m}{Dt}+\frac{7}{5}\frac{\partial u_a}{\partial x_a}q_m+\frac{7}{5}\frac{\partial u_m}{\partial x_a}q_a+\frac{2}{5}\frac{\partial u_a}{\partial x_m}q_a+\theta\frac{\partial p_{ma}}{\partial x_a}\\&+\frac{7}{2}p_{ma}\frac{\partial\theta}{\partial x_a}-\frac{p_{ma}}{\varrho}\frac{\partial\sigma_{ab}}{\partial x_b}+\frac{5}{2}p\frac{\partial\theta}{\partial x_m}=\frac{1}{\lambda}\Theta_m,\end{aligned}\tag{2.32}$$

where

$$\frac{1}{\lambda}\Theta_m=-C_1\frac{\widetilde{\sigma}}{\widetilde{m}}\sqrt[2]{\varrho}\sqrt[2]{I_1}q_m.\tag{2.33}$$

It is clear that Eq. (2.32) is different than the last equation in (2.18) (see Ref. 3).

We notice that Eq. (2.18) can effectively be derived from the truncated Boltzmann equation (2.4) with $\widehat{Q}_1$ in place of $\widehat{Q}$. Thus, it is natural to ask what is the "Boltzmann equation" that corresponds to this procedure. By taking the inverse Fourier transform of $\widehat{Q}_1$, it is not difficult to show that for hard spheres,

$$\frac{\partial f}{\partial t}+\xi\cdot\nabla_x f=\frac{16\pi}{\lambda}Q_1(f,f),\tag{2.34}$$

$$Q_1(f,f)=\frac{1}{3!}\Delta_\xi\int_{E^3}dw\,|w|^3\,F[\xi,w]-\sum_{|\alpha|=2}\frac{1}{\alpha!}\frac{\partial^\alpha}{\partial^\alpha\xi}\int_{E^3}dw\,|w|\,w^\alpha F[\xi,w],$$

where

$$F[\xi,w]=f[\xi+w]\,f[\xi-w].\tag{2.35}$$

Consequently, we arrive at Landau-like approximation of the collision kernel that, in spirit, is similar to Villani's result on the Landau equation (see Ref. 24 for extensive list of references).

3. LEVERMORE 14 MOMENT DENSITY

In this section we examine Levermore's 14 moment approximation of the density $F_\Lambda[v]$, $v\epsilon E^3$ (see Ref. 16). We are interested in a quantified description of that density so it could be compared with the 13 moment approximation describe in Sec. 2. In order to explain our idea, we start with a one-dimensional caricature of the original problem. We examine one-dimensional density $F_\Lambda[v]$ given by the formula (see Ref. 14),

$$\begin{aligned}F_\Lambda[v]&=e^{-A[v]},\quad v\epsilon R,\\A[v]&=A_0+A_1v+A_2v^2+A_3v^3+A_4v^4.\end{aligned}\tag{3.1}$$

We wish to identify the unknown coefficients A_n through the set of conditions for the prescribed densities ρ_n,

$$\varrho_n = \int_{\mathrm{R}} dv v^n e^{-A[v]}, \quad n = 0, 1, 2, 3, 4. \tag{3.2}$$

By introducing a convex Godunov potential (see Refs. 8, 15, 16),

$$G = \int_{\mathrm{R}} dv e^{-A[v]}, \tag{3.3}$$

and by computing,

$$\varrho_n = -\frac{\partial G}{\partial A_n}, \quad n = 0, 1, 2, 3, 4, \tag{3.4}$$

one can show that Eq. (3.2) have a unique solution for A_n's in terms of ϱ_n's. By analogy with the three-dimensional problem, we call ρ_0 and $u = \varrho_{1/}\varrho_0$ the "macroscopic density ϱ" and the "macroscopic velocity u."

The macroscopic velocity u defines the centered density,

$$f_\Lambda [\xi] = F_\Lambda [\xi + u], \tag{3.5}$$

in terms of the peculiar velocity $\xi = v - u$. The new density $f_\Lambda [\xi]$ defines a new sequence of centered moments σ_n that are given by the integrals,

$$\sigma_n = \int_{\mathrm{R}} d\xi \xi^n f_\Lambda [\xi], \quad n = 0, 1, 2, 3, 4. \tag{3.6}$$

Comparing ϱ_n's with σ_n's we see that $\sigma_1 = 0$ and

$$\begin{aligned}
\varrho_0 &= \sigma_0, \\
\varrho_1 &= \sigma_0 u, \\
\varrho_2 &= \sigma_0 u^2 + \sigma_2, \\
\varrho_3 &= \sigma_0 u^3 + 3u\sigma_2 + \sigma_3, \\
\varrho_4 &= \sigma_0 u^4 + 6u^2\sigma_2 + 4u\sigma_3 + \sigma_4.
\end{aligned} \tag{3.7}$$

Hence, the mapping defined by Eq. (3.7),

$$[\sigma_0, u, \sigma_2, \sigma_3, \sigma_4] \longrightarrow [\varrho_0, \varrho_1, \varrho_2, \varrho_3, \varrho_4], \tag{3.8}$$

is 1:1 and "onto" with an inverse that can explicitly be computed.

We wish to show that $f_\Lambda [\xi]$ is independent of u. First of all, we notice that

$$\begin{aligned}
f_\Lambda [\xi] &= F_\Lambda [\xi + u] = e^{-B[\xi]}, \\
B [\xi] &= B_0 + B_1\xi + B_2\xi^2 + B_3\xi^3 + B_4\xi^4,
\end{aligned} \tag{3.9}$$

where,

$$\begin{aligned} B_0 &= A_0 + A_1 u + A_2 u^2 + A_3 u^3 + A_4 u^4, \\ B_1 &= A_1 + 2A_2 u + 3A_3 u^2 + 4A_4 u^3, \\ B_2 &= A_2 + 3A_3 u + 6A_4 u^2, \\ B_3 &= A_3 + 4A_4 u, \\ B_4 &= A_4. \end{aligned} \tag{3.10}$$

Thus, for all u,

$$\mathbf{B} = \mathcal{L}[u]\,\mathbf{A}, \qquad Det\mathcal{L}[u] = 1. \tag{3.11}$$

Now, we define a new Godunov potential,

$$G^* = \int_{\mathrm{R}} d\xi e^{-B[\xi]} = \int_{\mathrm{R}} d\xi\ f_\Lambda[\xi], \tag{3.12}$$

where, in view of Eq. (3.11), B_0, B_1, B_2, B_3, B_4 are independent variables. As before, we obtain a sequence of equations that is valid for all u's,

$$\sigma_0 = -\frac{\partial G^*}{\partial B_0}, \quad \sigma_1 = 0 = -\frac{\partial G^*}{\partial B_1}, \quad \sigma_n = -\frac{\partial G^*}{\partial B_n}, \quad n = 2, 3, 4. \tag{3.13}$$

Next, in Eq. (3.4) we set $u = 0$ or equivalently $\varrho_1 = 0$,

$$\varrho_0 = -\frac{\partial G}{\partial A_0}, \quad 0 = -\frac{\partial G}{\partial A_1}, \quad \varrho_n = -\frac{\partial G}{\partial A_n}, \quad n = 2, 3, 4. \tag{3.14}$$

But for $u = 0$, Eq. (3.7) imply that $\varrho_n = \sigma_n$ for all n. Consequently, Eq. (3.13) are identical with Eq. (3.14) except for the name of variables that appear in G and G^*. By existence and uniqueness of A_n's we conclude that for all values of u and n,

$$B_n = A_n[\varrho_0, 0, \varrho_2, \varrho_3, \varrho_4] = A_n[\sigma_0, 0, \sigma_2, \sigma_3, \sigma_4]. \tag{3.15}$$

Inverting Eq. (3.10) we see that A_n's are prescribed polynomials in u, with the coefficients that depend on $\sigma_0, \sigma_2, \sigma_3, \sigma_4$ alone,

$$\begin{aligned} A_0 &= B_0 - B_1 u + B_2 u^2 - B_3 u^3 + B_4 u^4, \\ A_1 &= B_1 - 2B_2 u + 3B_3 u^2 - B_4 u^3, \\ A_2 &= B_2 - 3B_3 u - 6B_4 u^2, \\ A_3 &= B_3 - 4B_4 u, \\ A_4 &= B_4. \end{aligned} \tag{3.16}$$

Therefore, the problem of finding A_n's from Eq. (3.2) can be reduced to the problem of finding B_0, B_1, B_2, B_3, B_4 from the following set of equations,

$$f_\Lambda [\xi] = e^{-B[\xi]}, \quad B[\xi] = B_0 + B_1\xi + B_2\xi^2 + B_3\xi^3 + B_4\xi^4, \tag{3.17}$$

where,

$$\begin{aligned} &\varrho = \int_{\mathrm{R}} d\xi f_\Lambda [\xi], \qquad 0 = \int_{\mathrm{R}} d\xi\xi\, f_\Lambda [\xi], \\ &\varrho\theta = \int_{\mathrm{R}} d\xi\xi^2 f_\Lambda [\xi], \quad \varrho\chi = \int_{\mathrm{R}} d\xi\xi^3 f_\Lambda [\xi], \quad \varrho\mu = \int_{\mathrm{R}} d\xi\xi^4 f_\Lambda [\xi]. \end{aligned} \tag{3.18}$$

The conventional symbols θ, χ, can be identified with the "temperature" and with the "heat flux" per unit density, while the moment μ must remain nameless as it has no macroscopic analogue in the classical gas dynamics.

The arguments presented above can be applied, almost verbatim, to all densities that appear in Levermore's work.(16) Therefore the entropies,

$$h_\Lambda = \int_{\mathrm{E}^3} dv\, [F_\Lambda [v] \ln (F_\Lambda [v]) - F_\Lambda [v]] = \int_{\mathrm{E}^3} d\xi\, [f_\Lambda [\xi] \ln (f_\Lambda [\xi]) - f_\Lambda [\xi]], \tag{3.19}$$

associated with those densities are independent of $u \epsilon \mathrm{E}^3$ (see Ref. 19).

Next, we consider Levermore's 14 moment density $F_\Lambda [v]$,

$$\begin{aligned} &F_\Lambda[v] = e^{-A[v]}, \quad v\epsilon\mathrm{E}^3, \\ &A[v] = B_0^* + \langle L^*|v\rangle + \frac{1}{2}\langle M^*v|v\rangle + \langle N^*|v\rangle\langle v|v\rangle + W_0^*\langle v|v\rangle^2. \end{aligned} \tag{3.20}$$

By repeating the arguments for one-dimensional case, we reduce the problem of finding $F_\Lambda[v]$ to the problem of finding the centered density $f_\Lambda[\xi]$, such that $F_\Lambda[v] = f_\Lambda[v - u]$. The new density has the form,

$$\begin{aligned} &f_\Lambda [\xi] = e^{-B[\xi]}, \quad \xi\epsilon\mathrm{E}^3, \\ &B[\xi] = B_0 + \langle L|\,\xi\rangle + \frac{1}{2}\langle M\xi|\,\xi\rangle + \langle N|\,\xi\rangle\,\langle\xi|\,\xi\rangle + W_0\,\langle\xi|\,\xi\rangle^2. \end{aligned} \tag{3.21}$$

The 14 unknown functions, $B_0, L_a, M_{ab}, N_a, W_0$ must be found from 14 conditions on the moments of $f_\Lambda [\xi]$,

$$\begin{aligned} &\varrho = \int_{\mathrm{E}^3} d\xi\, f_\Lambda [\xi], \quad 0 = \int_{\mathrm{E}^3} d\xi\xi_a\, f_\Lambda [\xi], \quad \varrho\theta_{ab} = \int_{\mathrm{E}^3} d\xi\xi_a\xi_b\, f_\Lambda [\xi], \\ &\varrho\chi_a = \int_{\mathrm{E}^3} d\xi\xi_a\,\langle\xi|\,\xi\rangle\, f_\Lambda [\xi], \quad \varrho\mu = \int_{\mathrm{E}^3} d\xi\,\langle\xi|\,\xi\rangle^2 f_\Lambda [\xi]. \end{aligned} \tag{3.22}$$

As in Sec. 1, we study Fourier transform of $f_\Lambda[\xi]$,

$$\widehat{f_\Lambda}[k] = \int_{E^3} d\xi e^{-i\langle k|\xi\rangle} f_\Lambda[\xi], \tag{3.23}$$

that corresponds to $\widehat{f_\Lambda}[k, \rho_*, \theta_*, \chi_*, \mu_*]$ from Eq. (2.12). The standard formula,

$$i^{|\alpha|+|\beta|}\partial^\alpha\left[k^\beta \widehat{f}[k]\right] = \mathcal{F}\left[\xi^\alpha \partial^\beta f[\xi]\right], \tag{3.24}$$

together with Eq. (3.22) implies that

$$\begin{aligned}\widehat{f_\Lambda}[0] = \varrho, \quad \partial_a \widehat{f_\Lambda}[0] = 0, \quad \partial_a\partial_b \widehat{f_\Lambda}[0] = -\varrho\theta_{ab},\\ \partial_a \Delta \widehat{f_\Lambda}[0] = i\varrho\chi_a, \qquad \Delta^2 \widehat{f_\Lambda}[0] = \varrho\mu.\end{aligned} \tag{3.25}$$

Since $f_\Lambda[\xi] = e^{-B[\xi]}$,

$$\partial_a f_\Lambda[\xi] + \partial_a B[\xi] f_\Lambda[\xi] = 0. \tag{3.26}$$

Using Eq. (3.24), we compute the Fourier transform of the last equation. We obtain a system of 3 partial differential equations with 14 “initial conditions” (3.25),

$$\begin{aligned}i4W_0\partial_a\Delta\widehat{f_\Lambda}[k] + 2N_s\partial_s\partial_a\widehat{f_\Lambda}[k] = ik_a\widehat{f_\Lambda}[k] + L_a\widehat{f_\Lambda}[k] + iM_{as}\partial_s\widehat{f_\Lambda}[k]\\ - N_a\Delta\widehat{f_\Lambda}[k].\end{aligned} \tag{3.27}$$

Now, we differentiate Eq. (3.23): If π stands for any independent moment $\varrho, \theta_{ab}, \chi_a, \mu$ then,

$$\begin{aligned}-\frac{\partial}{\partial\pi}\widehat{f_\Lambda}[k] = \int_{E^3} d\xi e^{-i\langle k|\xi\rangle} e^{-B[\xi]}\\ \times\left[\frac{\partial B_0}{\partial\pi} + \frac{\partial L_a}{\partial\pi}\xi_a + \frac{1}{2}\frac{\partial M_{ab}}{\partial\pi}\xi_a\xi_b + \frac{\partial N_a}{\partial\pi}\xi_a\xi_b\xi_b + \frac{\partial W_0}{\partial\pi}\xi_a\xi_a\xi_b\xi_b\right].\end{aligned} \tag{3.28}$$

Eq. (3.28) yield a system of 11 equations for the 14 unknown functions, $B_0, L_a, M_{ab}, N_a, W_0$,

$$\begin{aligned}-\frac{\partial}{\partial\pi}\widehat{f_\Lambda}[k] = \widehat{f_\Lambda}[k]\frac{\partial B_0}{\partial\pi} + i\partial_a\widehat{f_\Lambda}[k]\frac{\partial L_a}{\partial\pi}\\ -\frac{1}{2}\partial_a\partial_b\widehat{f_\Lambda}[k]\frac{\partial M_{ab}}{\partial\pi} - i\partial_a\Delta\widehat{f_\Lambda}[k]\frac{\partial N_a}{\partial\pi} + \Delta^2\widehat{f_\Lambda}[k]\frac{\partial W_0}{\partial\pi}.\end{aligned} \tag{3.29}$$

Furthermore, Eq. (3.29) must be supplied with its own continuity conditions: by the uniqueness of Levermore’s construction, the moments computed for the Gaussian,

$$f_\Lambda[\xi] = \frac{\varrho}{[2\pi \det\theta]^{\frac{1}{2}}}\exp\left(-\frac{1}{2}\langle\theta^{-1}\xi\,|\xi\rangle\right), \tag{3.30}$$

and substituted into Eq. (3.22), must yield the Gaussian itself. Therefore, when

$$\varrho = \varrho, \quad \theta_{ab} = \theta_{ab}, \quad \chi_a = 0, \quad \mu = 2\theta_{ab}\theta_{ab} + \theta_{aa}\theta_{bb}, \tag{3.31}$$

we must have,

$$e^{-B_0} = \frac{\varrho}{[2\pi \det\theta]^{\frac{1}{2}}}, \quad L_a = 0, \quad M_{ab} = \left(\theta^{-1}\right)_{ab}, \quad N_a = 0, \quad W_0 = 0. \tag{3.32}$$

Consequently, we have 14 equations for the 14 unknown functions in Eq. (3.21). We can close our derivation by writing the formula for the entropy,

$$S = -\int_{\mathrm{E}^3} dv F_\Lambda[v] \ln F_\Lambda[v] = -\int_{\mathrm{E}^3} d\xi\, f_\Lambda[\xi] \ln f_\Lambda[\xi] = \int_{\mathrm{E}^3} d\xi\, e^{-B[\xi]} B[\xi],$$

$$S_\Lambda(\rho, \theta, \chi, \mu) = \varrho[B_0 + \frac{1}{2} M_{ab}\theta_{ab} + N_a\chi_a + W_0\mu]. \tag{3.33}$$

Any direct attempt to solve Eqs. (3.27), (3.29) by hand seems to be impractical. However, we may try to exploit Grad's expansion (1.27) to represent $f_\Lambda[k]$ as a power series in k. Unfortunately, it is impossible to test such an idea within confines of a single paper.

Nevertheless, it is possible to gain some insight into Levermore's problem by studying a one-dimensional density (see Ref. 13),

$$f_\Lambda[\xi] = \exp\left[-B_0 - B_2\xi^2 - B_4\xi^4\right], \tag{3.34}$$

where the functions B_0, B_2, B_4 are determined by the three conditions,

$$\varrho = \int_{\mathrm{R}} d\xi f_\Lambda[\xi], \quad \varrho\theta = \int_{\mathrm{R}} d\xi \xi^2 f_\Lambda[\xi], \quad \varrho\mu = \int_{\mathrm{R}} d\xi \xi^4 f_\Lambda[\xi]. \tag{3.35}$$

It is not difficult to show that one-dimensional caricature of Eqs. (3.27), (3.29) together with the analog of the "initial conditions" (3.25), (3.32) yields,

$$f[\xi] = \frac{\varrho}{\sqrt[2]{2\pi\theta}} \exp(-q[\eta]) \exp\left(-\frac{1}{2\theta}[1 - 4\eta b[\eta]]\xi^2 - b[\eta]\xi^4\right), \tag{3.36}$$

where $\eta = \mu\theta^{-2}$ is an independent variable and

$$q[\eta] = \eta b[\eta] + \int_3^\eta d\overline{\eta} b[\overline{\eta}]. \tag{3.37}$$

The function $b[\eta]$ is described by the first order differential equation,

$$\frac{db}{d\eta} = \frac{8[\eta - 1]b^2}{[3 - \eta + 4\eta[1 - \eta]b]}, \quad \lim_{\eta \to 3} b[\eta] = 0, \tag{3.38}$$

whose solution is not amenable to a simple analysis unless $b[\eta] \equiv 0$. However, as Professor H. Gingold pointed out, Eq. (3.38) does have other solutions; all of them violate the key condition of the Levermore scheme,

$$b[\eta] > 0 \ \ for\ all \ \ \eta > 0 \ \ unless \ \ \eta = 3. \tag{3.39}$$

EPILOGUE

For the sake of argument, let us assume that Hamburger formula (1.44) holds true. Then we must agree that $\widehat{f}[k]$ does not depend on the macroscopic velocity of the gas $u(t, x)$. Therefore, we must accept that u does not appear in the collision operator $\widehat{Q}\left[\widehat{f}, \widehat{f}\right]$ and that u appears on the left hand side of the Boltzmann equation alone. Moreover, the entropy integral,

$$S = -\int_{E^3} d\xi\, f \ln f,$$

cannot depend on u either. Therefore S is Galilean invariant in the sense of extended thermodynamics (see Ref. 19). Above argument will remain true for any weighted Taylor expansion that is convergent.

APPENDIX I. WEIGHTED TAYLOR FORMULA ON R^n

We consider n differential operators L_j acting on a complex function ϕ,

$$L_j\phi(k) = \partial_j\phi(k) + a_j(k)\phi(k), \quad 1 \leq j \leq n, \ k \in R^n. \tag{I.1}$$

We must assume that operators L_j commute,

$$L_jL_k - L_kL_j = \left[\partial_j a_k - \partial_k a_j\right] Id = 0. \tag{I.2}$$

Consequently, there exists a function $A(k)$ such that $a_j(k) = \partial_j A(k)$. For a given function ϕ, we set

$$f(k) = e^{A(k)}\phi(k), \quad k \in R^n, \tag{I.3}$$

and we check that for any multi index $\alpha = (\alpha_1, \ldots, \alpha_n)$,

$$\partial^\alpha f(k) = e^{A(k)} L^\alpha \phi(k), \quad L^\alpha = L_1^{\alpha_1} L_2^{\alpha_2} \cdots L_n^{\alpha_n}. \tag{I.4}$$

Next, we write down the Taylor formula for f in $C^{N+1}(R^n)$,

$$f(x+k) = \sum_{|\alpha| \leq N} \partial^\alpha f(x) \frac{k^\alpha}{\alpha!} + \sum_{|\alpha| = N+1} \frac{k^\alpha}{\alpha!} \int_0^1 ds\ [N+1][1-s]^N \partial^\alpha f(x+sk). \tag{I.5}$$

We substitute Eqs. (I.3), (I.4) into Eq. (I.5). Then the modified Taylor expansion for the function ϕ emerges as the formula,

$$\phi(x+k) = e^{A(x)-A(x+k)} \left[\sum_{|\alpha| \le N} L^{\alpha} \phi(x) \frac{k^{\alpha}}{\alpha!} + R_N(x,k) \right], \tag{I.6}$$

where,

$$R_N(x,k) = e^{-A(x)} \sum_{|\alpha|=N+1} \frac{k^{\alpha}}{\alpha!} \int_0^1 ds\ \ [N+1][1-s]^N e^{A(x+sk)} L^{\alpha} \phi(x+sk). \tag{I.7}$$

For $x = 0$ and $A(0) = 0$, we recover the McLaurin expansion that we use throughout the paper,

$$\begin{aligned} \phi(k) &= e^{-A(k)} \left[\sum_{|\alpha| \le N} L^{\alpha} \phi(0) \frac{k^{\alpha}}{\alpha!} + R_N(k) \right], \\ R_N(k) &= \sum_{|\alpha|=N+1} \frac{k^{\alpha}}{\alpha!} \int_0^1 ds\ \ [N+1][1-s]^N e^{A(sk)} L^{\alpha} \phi(sk). \end{aligned} \tag{I.8}$$

The formulae for the derivatives of ϕ, up to the third order, that are necessary to compute the 13 and the 20 moment approximation of the density $\widehat{f}(k)$ are as follows,

$$\begin{aligned} L_a \phi &= \partial_a \phi + \partial_a A \cdot \phi, \\ L_a L_b \phi &= \partial_a \partial_b \phi + \partial_a A \cdot \partial_b \phi + \partial_b A \cdot \partial_a \phi + [\partial_a \partial_b A + \partial_a A \cdot \partial_b A] \cdot \phi, \\ L_a L_b L_c \phi &= \partial_a \partial_b \partial_c \phi + \partial_a A \cdot \partial_b \partial_c \phi + \partial_b A \cdot \partial_a \partial_c \phi + \partial_c A \cdot \partial_a \partial_b \phi \\ &\quad + [\partial_a \partial_b A + \partial_a A \cdot \partial_b A] \cdot \partial_c \phi + [\partial_a \partial_c A + \partial_a A \cdot \partial_c A] \cdot \partial_b \phi \\ &\quad + [\partial_c \partial_b A + \partial_c A \cdot \partial_b A] \cdot \partial_a \phi + [\partial_a \partial_b \partial_c A + \partial_a \partial_c A \cdot \partial_b A \\ &\quad + \partial_a \partial_b A \cdot \partial_c A + \partial_b \partial_c A \cdot \partial_a A + \partial_a A \cdot \partial_b A \cdot \partial_c A] \cdot \phi. \end{aligned} \tag{I.9}$$

In Eq. (I.9), for the sake of brevity, we dropped the argument of ϕ and A.

We would like to add that the formula for $L_a L_b L_c L_n \phi$ contains over 50 terms. Therefore it is of great computational importance that $\partial_n A(0) = 0$. This is indeed the case, when we study the moments of the Boltzmann equation in terms of $\widehat{f}[k]$ and not $\widehat{F}[k]$.

APPENDIX II. PIZZETTI'S FORMULA

Inverse Fourier transform applied to $f[\xi]$ yields the formula,

$$f[\xi + s\,|p|\,n] = \int_{\mathrm{E}^3} \frac{dk}{[2\pi]^3} \exp[ik\cdot\xi] \exp[is\,|p|\,k\cdot n]\; \widehat{f}[k]. \tag{II.1}$$

We take the spherical average of both sides of Eq. (II.1) and we obtain,

$$\begin{aligned} \langle f[\xi + s\,|p|\,n]\rangle_{\mathrm{S}^2} &= \int_{\mathrm{S}^2} \frac{dn}{4\pi}\, f[\xi + s\,|p|\,n] \\ &= \int_{\mathrm{E}^3} \frac{dk}{[2\pi]^3} \exp[ik\cdot\xi] \frac{\sin[s\,|p|\,|k|]}{s\,|p|\,|k|}\, \widehat{f}[k]. \end{aligned} \tag{II.2}$$

A standard Taylor expansion implies that,

$$\begin{aligned} \frac{\sin[|p|\,|k|]}{|p|\,|k|} &= \sum_{m=0}^{M} \frac{|p|^{2m}}{[2m+1]!}\left[-|k|^2\right]^m \\ &+ \frac{|p|^{2M+2}}{[2M+2]!} \int_0^1 ds\,[1-s]^{2M+2}\left[-|k|^2\right]^{M+1} \cos[s\,|p|\,|k|]. \end{aligned} \tag{II.3}$$

We substitute the last identity into Eq. (II.2). The properties of the Fourier transform yield,

$$\begin{aligned} \langle f[\xi + |p|\,n]\rangle_{\mathrm{S}^2} &= \sum_{m=0}^{M} \frac{|p|^{2m}}{[2m+1]!} \Delta_\xi^m f[\xi] \\ &+ \frac{|p|^{2M+2}}{[2M+2]!} \int_0^1 ds\,[1-s]^{2M+2}\, \Delta_\xi^{M+1} F[\xi, s\,|p|], \\ F[\xi, s\,|p|] &= \int_{\mathrm{E}^3} \frac{dk}{[2\pi]^3} \exp[ik\cdot\xi] \cos[s\,|p|\,|k|]\; \widehat{f}[k]. \end{aligned} \tag{II.4}$$

Eq. (II.2) implies that,

$$\frac{d}{ds}[s\,\langle f[\xi + s\,|p|\,n]\rangle_{\mathrm{S}^2}] = F[\xi, s\,|p|]. \tag{II.5}$$

Consequently, after few simple manipulations, we arrive at the finite version of the Pizzetti's formula,

$$\begin{aligned} \langle f[\xi + |p|\,n]\rangle_{\mathrm{S}^2} &= \sum_{m=0}^{M} \frac{|p|^{2m}}{[2m+1]!} \Delta_\xi^m f[\xi] + O_M[\xi, |p|], \\ O_M[\xi, |p|] &= \frac{|p|^{2M+2}}{[2M+1]!} \int_0^1 ds\, s\;[1-s]^{2M+2} \left\langle \Delta_\xi^{M+1} f[\xi + s\,|p|\,n]\right\rangle_{\mathrm{S}^2}. \end{aligned} \tag{II.6}$$

In this paper we use Zalcman's version of the identity (II.6) with $M = \infty$ that appears in Ref. 25.

Eqs. (III.12), (II.2) yield an easy proof of the fact that Laplacian commutes with the operation of taking the spherical average. We can also recover the Euler–Poisson–Darboux's equation, that appears while studying the wave equation.

APPENDIX III. FOURIER TRANSFORM OF THE BOLTZMANN EQUATION

We consider a gas of rigid spheres that occupies a region D_x in E^3. The evolution of the gas is described by the Boltzmann equation for the unknown density $F(t, x, v)$ (see Ref. 4),

$$\frac{\partial F}{\partial t} + v \cdot \nabla_x F + g \cdot \nabla_v F = \frac{1}{\lambda} Q[F, F], \quad t > 0, \quad x \in D_x, \quad v \in \mathrm{E}^3, \tag{III.1}$$

with the collision operator $Q[F, F]$ given by the integral,

$$Q[F, F][v] = \frac{1}{4} \int_{\mathrm{E}^3} du\, |u| \int_{\mathrm{S}^2} dn \left[F\left[v_*^1\right] F\left[v^1\right] - F[v_*] F[v] \right]. \tag{III.2}$$

The pair $\left(v_*^1, v^1\right)$ describes the velocities of two spheres before their collision and the pair (v_*, v) represents their velocities thereafter. Since the collisions are elastic, both pairs are related by the formulas,

$$v_*^1 = v + \frac{1}{2} u + \frac{1}{2} |u|\, n, \quad v^1 = v - \frac{1}{2} u - \frac{1}{2} |u|\, n, \quad u = v - v_*, \tag{III.3}$$

the unit vector n being parallel to $u^1 = v^1 - v_*^1$. The integration with respect to n, relative to the ordinary surface measure dn, extends to the whole unit sphere S^2.

We introduce the Fourier transform of F with respect to v and we write the transformation's inverse,

$$\widehat{F}[k] = \int_{\mathrm{E}^3} dv e^{-i\langle k|v\rangle} F[v], \quad F[v] = \int_{\mathrm{E}^3} \frac{dk}{[2\pi]^3} e^{i\langle k|v\rangle} \widehat{F}[k]. \tag{III.4}$$

We also modify the collision operator Q by multiplying its integrand by $e^{-\varepsilon|u|}$,

$$Q_\varepsilon[F, F][\xi] = \frac{1}{4} \int_{\mathrm{E}^3} du e^{-\varepsilon|u|} |u| \int_{\mathrm{S}^2} dn \left[F\left[v_*^1\right] F\left[v^1\right] - F[v_*] F[v] \right]. \tag{III.5}$$

Next, we introduce the spherical change of variables,

$$u = mw, \quad du = w^2 dw\, dm, \quad m \in \mathrm{S}^2. \tag{III.6}$$

Upon this change, the collision operator Q_ε becomes an ordinary integral of a double spherical average over $S^2 \times S^2$,

$$Q_\varepsilon[F,F][v] = \frac{1}{4}\int_0^\infty dw e^{-\varepsilon|w|}\,|w|^3$$
$$\times \int_{S^2\times S^2} dn\,dm \left[F\left[v_*^1\right]F\left[v^1\right] - F\left[v_*\right]F\left[v\right]\right]. \quad \text{(III.7)}$$

Now, we substitute the integral for the inverse Fourier transform of $\widehat{F}$ into the formula for Q_ε. Using the properties of the Fourier transform and the formula

$$\int_{S^2} dn\, e^{i\langle q|n\rangle} = 4\pi\frac{\sin(|q|)}{|q|}, \quad \text{(III.8)}$$

we obtain that,

$$Q_\varepsilon[F,F][v] = \int_{E^3}\frac{dk}{[2\pi]^3}e^{i\langle k|v\rangle}\,\widehat{Q}_\varepsilon[\widehat{F},\widehat{F}][k]. \quad \text{(III.9)}$$

The new collision operator $\widehat{Q}_\varepsilon[\widehat{F},\widehat{F}]$ has the following form,

$$\widehat{Q}_\varepsilon[\widehat{F},\widehat{F}][k] = \frac{1}{\pi}\int_{E^3} dz\,\widehat{F}\left[\frac{1}{2}k+\frac{1}{2}z\right]\widehat{F}\left[\frac{1}{2}k-\frac{1}{2}z\right]\Delta_z S_\varepsilon(k,z). \quad \text{(III.10)}$$

The kernel $S_\varepsilon(k,z)$ is given by the Laplace integral,

$$S_\varepsilon(k,z) = \int_0^\infty dw\,e^{-\varepsilon w}\left[\frac{1}{2}\left[\frac{\sin(|k+z|\,w)}{|k+z|}+\frac{\sin(|k-z|\,w)}{|k-z|}\right]\right.$$
$$\left. -\frac{\sin(|k|\,w)\sin(|z|\,w)}{|k|\,|z|\,w}\right]. \quad \text{(III.11)}$$

The Laplace operator Δ_z appears in $\widehat{Q}_\varepsilon$ as the result of the key identity for the Helmholtz equation in E^3, applied to the spherical averages that emerge while computing $Q_\varepsilon[F,F]$ in terms of $\widehat{F}$,

$$h(z) = -\frac{1}{A^2}\Delta_z h(z), \quad h(z) = \frac{\sin(A\,|z-c|)}{A\,|z-c|}, \qquad z\in E^3. \quad \text{(III.12)}$$

Although the kernel $S_\varepsilon(k,z)$ makes no sense without the factor $e^{-\varepsilon w}$, the kernel $S_\varepsilon(k,z)$ can explicitly be evaluated,

$$S_\varepsilon(k,z) = \frac{1}{2}\left[\frac{1}{|k+z|^2+\varepsilon^2}+\frac{1}{|k-z|^2+\varepsilon^2}\right]$$
$$-\frac{1}{2}\left[\left\langle\frac{1}{|k+z|^2+\varepsilon^2}\right\rangle_{S^2}+\left\langle\frac{1}{|k-z|^2+\varepsilon^2}\right\rangle_{S^2}\right]. \quad \text{(III.13)}$$

The symbol $\langle A(x)\rangle_{S^2}$ stands for the normalized, spherical average of a function $A(x)$ over the unit sphere,

$$\langle A(x)\rangle_{S^2} = \frac{1}{4\pi}\int_{S^2} dn\, A(|x|\, n)\,. \tag{III.14}$$

Consequently, integrating formula (III.10) by parts and letting ε go to 0, we arrive at the sequence of relations, that yields the Fourier transform of Q,

$$\begin{aligned} Q[F,F][v] &= \lim_{\varepsilon\to 0} Q_\varepsilon[F,F][v] \\ &= \int_{E^3} \frac{dk}{2\pi^3} e^{i\langle k|v\rangle} \lim_{\varepsilon\to 0} \widehat{Q}_\varepsilon[\widehat{F},\widehat{F}][k] = \int_{E^3} \frac{dk}{2\pi^3} e^{i\langle k|v\rangle}\, \widehat{Q}[\widehat{F},\widehat{F}][k]\,. \end{aligned} \tag{III.15}$$

It is easy to see that, the new collision operator $\widehat{Q}$ is given by the integral,

$$\begin{aligned} &\widehat{Q}[\widehat{F},\widehat{F}][k] = \frac{1}{\pi}\int_{E^3} dz\, S(k,z)\ \Psi[k,z]\,, \\ &\quad \Psi[k,z] = \Delta_z \Phi[k,z]\,, \quad \Phi[k,z] = \widehat{F}\left[\frac{1}{2}k + \frac{1}{2}z\right]\widehat{F}\left[\frac{1}{2}k - \frac{1}{2}z\right], \\ &\lim_{\varepsilon\to 0} S_\varepsilon(k,z) = S(k,z) = \frac{1}{2}\left[\frac{1}{|k+z|^2} + \frac{1}{|k-z|^2}\right] \\ &\qquad\qquad -\frac{1}{2}\left[\left\langle\frac{1}{|k+z|^2}\right\rangle_{S^2} + \left\langle\frac{1}{|k-z|^2}\right\rangle_{S^2}\right]. \end{aligned} \tag{III.16}$$

Therefore, the Fourier transform of the Boltzmann equation has the following form,

$$\frac{\partial \widehat{F}}{\partial t} + i\nabla_x \cdot \nabla_k \widehat{F} + ig\cdot k\widehat{F} = \frac{1}{\lambda}\widehat{Q}[\widehat{F},\widehat{F}]. \tag{III.17}$$

The original Boltzmann equation is supplied with the standard boundary condition (see Ref. 4): If e is the inner, unit normal at $x \in \partial D_x$ then for all v such that $\langle v|\, e\rangle > 0$,

$$\langle e|\, v\rangle\, F[v] + \int_{\langle e|v^*\rangle<0} dv^* R[v^*\,|v]\ \langle e|\, v^*\rangle F[v^*] = 0. \tag{III.18}$$

The kernel $R[v^*\,|v]$ is positive and its integral is equal to 1, that is,

$$\int_{\langle e|v\rangle>0} dv R[v^*\,|v] = 1. \tag{III.19}$$

To compute the Fourier transform of the boundary condition (III.18), we introduce the Heaviside step function,

$$H(s) = \begin{cases} 1 \text{ if } s > 0, \\ 0 \text{ if } s \le 0, \end{cases} \tag{III.20}$$

and we replace Eq. (III.18) by its modified variant, that is valid for all v's,

$$\begin{aligned} & H(\langle e|\, v\rangle)\, \langle e|\, v\rangle\, F[v] + \int_{E^3} dv^* P[v^*\,|v]\, \langle e|\, v^*\rangle F[v^*] = 0, \\ & P[v^*\,|v] = H(-\langle e|\, v^*\rangle)\, R[v^*\,|v]\, H(\langle e|\, v\rangle). \end{aligned} \tag{III.21}$$

It is not difficult to compute the Fourier transform of Eq. (III.21) in the sense of distributions. Routine computations yield,

$$\begin{aligned} & \int_{E^3} dp\ \langle e|\, \nabla_k \widehat{F}[k-p]\rangle \widehat{H}(p) + \int_{E^3} dp\ \langle e|\, \nabla_k \widehat{F}[p]\rangle\, \widehat{P}[-p\,|k] = 0, \\ & \widehat{P}[a^*\,|b] = \int_{E^3 \times E^3} dv^* dv\, e^{-i\langle a^*|v^*\rangle} e^{-i\langle b|v\rangle}\ P[v^*\,|v]. \end{aligned} \tag{III.22}$$

The tempered distribution $\widehat{H}$ is defined by its action on a test function ϕ by the formula,

$$\int_{E^3} dp\, \widehat{H}(p)\, \phi[p] = 4\pi^3 \left[\phi[0] - \frac{i}{\pi} \int_0^\infty ds \frac{\phi[s,0,0] - \phi[-s,0,0]}{s} \right], \tag{III.23}$$

providing that at $x \in \partial D_x$ we choose a local, orthonormal system of coordinates such that $v = v_1 e + v_2 e_2 + v_3 e_3$. We notice that Eqs. (III.17), (III.22) define the boundary value problem for the Boltzmann equation in terms of $\widehat{F}(t, x, k)$ alone.

The formula for the Fourier transform of the Boltzmann equations that can be found in Refs. 1 and 24 is semi-explicit. It contains a distributional Fourier transform of the collision kernel B that still has to be evaluated. In E^3, this task can be completed by computing the integral,

$$\langle T\,|\phi\rangle = \int_{E^3} d\xi \int_{E^3} dw\ |\xi|^\gamma\, e^{-i\langle \xi|w\rangle} \phi[w], \quad 0 < \gamma \le 1. \tag{III.24}$$

In order to do so, we introduce the factor $e^{-\varepsilon|\xi|}$ and we pass with ξ to spherical coordinates,

$$\begin{aligned} \langle T_\varepsilon\,|\phi\rangle &= \int_{E^3} dw \int_{E^3} d\xi\, e^{-\varepsilon|\xi|}\, |\xi|^\gamma\, e^{-i\langle \xi|w\rangle} \phi[w] \\ &= \int_{E^3} dw \int_0^\infty d|\xi|\ e^{-\varepsilon|\xi|}\, |\xi|^{\gamma+2}\, 4\pi \frac{\sin[|\xi|\,|w|]}{|\xi|\,|w|} \phi[w]. \end{aligned} \tag{III.25}$$

Next, using identity (III.12), we write,

$$\langle T_\varepsilon \, | \phi \rangle = -4\pi \int_{\mathrm{E}^3} dw \frac{1}{|w|} \Delta_w \phi\, [w] \int_0^\infty d\, |\xi| \; e^{-\varepsilon |\xi|} \, |\xi|^{\gamma - 1} \sin\left[|\xi| \, |w| \right]. \tag{III.26}$$

The last integral can explicitly be computed,

$$\int_0^\infty dx\, e^{-\varepsilon x} x^{\gamma-1} \sin\left[x\, |w|\right] = \frac{\Gamma\,[\gamma]}{\left[\varepsilon^2 + |w|^2\right]^{\frac{\gamma}{2}}} \sin\left[\gamma \arctan\left[\frac{|w|}{\varepsilon}\right]\right]. \tag{III.27}$$

Hence, by taking $\varepsilon \to 0$ we conclude that,

$$\langle T \, | \phi \rangle = -4\pi \Gamma\,[\gamma] \sin\left[\frac{\pi}{2}\gamma\right] \int_{\mathrm{E}^3} dw \frac{1}{|w|^{1+\gamma}} \Delta_w \phi\, [w]. \tag{III.28}$$

APPENDIX IV. INVARIANTS AND EXPANSION OF THE COLLISION OPERATOR

The analogue of the collision invariants for the collision operator Q is the set of relations,

$$\widehat{Q}[\widehat{F}, \widehat{F}]\,[0] = 0, \qquad \nabla_k \widehat{Q}[\widehat{F}, \widehat{F}]\,[0] = 0, \qquad \Delta_k \widehat{Q}[\widehat{F}, \widehat{F}]\,[0] = 0. \tag{IV.1}$$

A direct differentiation under the sign of integral (III.16) produces apparent singularity of $\mathrm{S}\,(k, z)$ that are not locally integrable in E^3. We can, however, change the form of $\widehat{Q}$ to make such a differentiation possible. In order to do so, we apply the shifts by $+k$, $-k$ to the first two terms in the integral (III.16),

$$\begin{aligned} &\int_{\mathrm{E}^3} dz \, \frac{1}{2} \left[\frac{1}{|k+z|^2} + \frac{1}{|k-z|^2} \right] \Psi\,[k, z] \\ &\quad = \int_{\mathrm{E}^3} \frac{dw}{|w|^2} \frac{1}{2} \left[\Psi\,[k, w-k] + \Psi\,[k, w+k] \right]. \end{aligned} \tag{IV.2}$$

Then, in the remaining two terms we combine the integral identity,

$$\int_{\mathrm{E}^3} dz \; \langle A\,[z] \rangle_{\mathrm{S}^2} \; B\,[z] = \int_{\mathrm{E}^3} dz \, A\,[z] \; \langle B\,[z] \rangle_{\mathrm{S}^2}, \tag{IV.3}$$

with the explicit formula for the two spherical averages that appear in $\mathrm{S}\,(k, z)$,

$$\left\langle \frac{1}{|k \pm z|^2} \right\rangle_{\mathrm{S}^2} = \frac{1}{4\pi} \int_{\mathrm{S}^2} dn \frac{1}{||k|\, n \pm z|^2}. \tag{IV.4}$$

Shifting the resulting integrands again, we arrive at the expression,

$$\int_{E^3} dz \, \frac{1}{2} \left[\left\langle \frac{1}{|k+z|^2} \right\rangle_{S^2} + \left\langle \frac{1}{|k-z|^2} \right\rangle_{S^2} \right] \Psi[k, z]$$

$$= \int_{E^3} \frac{dw}{|w|^2} \int_{S^2} \frac{dn}{4\pi} \frac{1}{2} \left[\Psi[k, w - |k|\, n] + \Psi[k, w + |k|\, n] \right]. \qquad \text{(IV.5)}$$

Integrals (IV.2) and (IV.5) yield an alternative form of $\widehat{Q}$,

$$\widehat{Q}[\widehat{F}, \widehat{F}][k] = \frac{1}{\pi} \int_{E^3} \frac{dw}{|w|^2} \frac{1}{2} \left[\Psi[k, w - k] + \Psi[k, w + k] \right]$$

$$- \frac{1}{\pi} \int_{E^3} \frac{dw}{|w|^2} \int_{S^2} \frac{dn}{4\pi} \frac{1}{2} \left[\Psi[k, w - |k|\, n] + \Psi[k, w + |k|\, n] \right]. \quad \text{(IV.6)}$$

In Eq. (IV.6) the first integrand can be expanded into an ordinary Taylor series,

$$\frac{1}{2} \left[\Psi[k, w - k] + \Psi[k, w + k] \right] = \Psi[k, w] + \sum_{N=1}^{\infty} \sum_{|\alpha| = 2N} \frac{k^\alpha}{\alpha!} \frac{\partial^\alpha \Psi}{\partial^\alpha w} [k, w]. \qquad \text{(IV.7)}$$

The second integrand can be expanded similarly, using Pizzetti's formula that is described in Appendix II,

$$\frac{1}{4\pi} \int_{S^2} dn \, G[w + |k|\, n] = G[w] + \sum_{N=1}^{\infty} \frac{|k|^{2N}}{[2N+1]!} \Delta_w^N G[w]. \qquad \text{(IV.8)}$$

Consequently,

$$\int_{S^2} \frac{dn}{4\pi} \frac{1}{2} \left[\Psi[k, w - |k|\, n] + \Psi[k, w + |k|\, n] \right]$$

$$= \Psi[k, w] + \sum_{N=1}^{\infty} \frac{|k|^{2N}}{[2N+1]!} \Delta_w^N \Psi[k, w]. \qquad \text{(IV.9)}$$

Expansions (IV.7), (IV.9) yield a series expansion of $\widehat{Q}$,

$$\widehat{Q}[\widehat{F}, \widehat{F}][k] = \frac{1}{\pi} \int_{E^3} \frac{dw}{|w|^2}$$

$$\times \sum_{N=1}^{\infty} \left[\sum_{|\alpha| = 2N} \frac{k^\alpha}{\alpha!} \frac{\partial^\alpha \Psi}{\partial^\alpha w} [k, w] - \frac{|k|^{2N}}{[2N+1]!} \Delta_w^N \Psi[k, w] \right]$$

$$= \sum_{N=1}^{\infty} \frac{1}{\pi} \int_{E^3} \frac{dw}{|w|^2} \left[\sum_{|\alpha| = 2N} \frac{k^\alpha}{\alpha!} \frac{\partial^\alpha \Psi}{\partial^\alpha w} [k, w] - \frac{|k|^{2N}}{[2N+1]!} \Delta_w^N \Psi[k, w] \right]. \quad \text{(IV.10)}$$

Eq. (IV.10) contains monomials of even order alone. Hence, it is obvious that the first two conditions (IV.1) are trivially true. A simple differentiation of the first term in Eq. (IV.10) yields the third condition (IV.1).

For the future reference, we would like to point out that the collision invariants of $\widehat{Q}$ are independent of the nature and the origin of the function $\Psi\,[k, w]$. In other words, conditions (IV.1) do not depend on the fact that,

$$\Psi\,[k, w] = \Delta_w \Phi\,[k, w]\,, \quad \Phi\,[k, w] = \widehat{F}\left[\frac{1}{2}k + \frac{1}{2}w\right]\widehat{F}\left[\frac{1}{2}k - \frac{1}{2}w\right]. \qquad \text{(IV.11)}$$

Thus, any approximation of $\widehat{F}$ substituted into Boltzmann equation (III.17) will preserve the structure of the macroscopic balance laws, that are the well known consequence of the conditions (IV.1).

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